

```
ring/chain bonds :
    2-3
exact/norm bonds :
    1-2 2-3 3-4

Match level :
    1:CLASS 2:CLASS 3:CLASS 4:CLASS
```

1 4

ring/chain nodes : 2 3 chain bonds : 1-2 3-4

## => d his

(FILE 'HOME' ENTERED AT 16:07:44 ON 19 FEB 2006) FILE 'REGISTRY' ENTERED AT 16:07:49 ON 19 FEB 2006 L1375 S SUCCINONITRILE L21 S SUCCINONITRILE/CN L3 STRUCTURE UPLOADED L450 S L3 L5 66602 S 5-7/SZ L6 2228 S C3N2-C5N2/EA FILE 'CAPLUS' ENTERED AT 16:11:41 ON 19 FEB 2006 2546 S L1 L7 1465 S L6 L8 L9 2 S L7 AND L8 FILE 'REGISTRY' ENTERED AT 16:12:33 ON 19 FEB 2006 3703 S L3 SSS FUL L10 FILE 'CAPLUS' ENTERED AT 16:12:41 ON 19 FEB 2006 4057 S L10 L11 L12 3 S L8 AND L11 L13 1 S L12 NOT L9 FILE 'REGISTRY' ENTERED AT 16:15:13 ON 19 FEB 2006 L14 STRUCTURE UPLOADED L15 50 S L14 L16 41797 S L14 SSS FUL FILE 'CAPLUS' ENTERED AT 16:15:52 ON 19 FEB 2006 24741 S L16 L17

=> d ibib abs hitstr total

8 S L8 AND L17

L18

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10/734,545
    ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:
                           2006:99766 CAPLUS
                           STAT3 decoy oligonucleotides and use in the treatment
                           of cancer
INVENTOR (S):
                           Grandis, Jennifer, Rubin; Johnson, Daniel, E.; Leong,
                           Paul
PATENT ASSIGNEE(S):
                           University of Pittsburgh - Of the Commonwealth System
                           of Higher Education, USA
SOURCE:
                           PCT Int. Appl., 67 pp.
                           CODEN: PIXXD2
DOCUMENT TYPE:
                           Patent
LANGUAGE:
                           English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                           KIND
                                   DATE
                                               APPLICATION NO.
                                                                          DATE
                           ----
                                                -----
     ______
                                   _____
     WO 2006012625
                            A2
                                   20060202
                                              WO 2005-US26361
                                                                          20050722
          W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
              LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
              NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
              SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
              ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:
                                                US 2004-590747P
                                                                      P 20040722
     A composition is provided that is useful in treating cancers in which STAT3 is
AB
     activated, such as squamous cell carcinomas including squamous cell
     carcinoma of the head and neck. The composition comprises an effective amount
of
     a STAT3 decoy and a pharmaceutically acceptable carrier. Also provided
     are methods of treating such cancers and methods of modulating STAT3
     transcriptional activation in a cell.
     INDEXING IN PROGRESS
IT
     53910-25-1, Pentostatin 109511-58-2
IT
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
         (STAT3 decoy oligonucleotides and use in treatment of cancer)
     53910-25-1 CAPLUS
RN
```

Imidazo [4,5-d] [1,3] diazepin-8-ol,  $3-(2-\text{deoxy}-\beta-D-\text{erythro}-\beta-D-\text{erythro})$ 

pentofuranosyl)-3,4,7,8-tetrahydro-, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CN

L18 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:759869 CAPLUS

DOCUMENT NUMBER: 141:243771

TITLE: Process for the stereoselective synthesis of

pentostatin aglycon and pentostatin via cyclization of

dinitrile derivatives with amines

INVENTOR(S):
Sourena, Nadji; Smoot, James; Sampath, Umashanker

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 21 pp.

CODEN: USXXCO

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
US 2004181052	<b>A1</b>	20040916	US 2003-734545	20031212		
PRIORITY APPLN. INFO.:			US 2002-432380P P	20021212		

OTHER SOURCE(S): MARPAT 141:243771

GI

AB A novel, scalable and improved process for preparing pentostatin and its analogs via stereoselective cyclization is disclosed. The method comprises the diastereospecific synthesis of the nucleobase from com. available L-dialkyl tartrate. Cyclization of dinitrile derivs., e.g. I, with a number of amines, e.g. allylamine, was performed to examine the practicality of the formation of the imidazole ring via the nucleophilic addition of an amino group to an electrophilic cyano functionality.

TT 749917-70-2P 749917-71-3P 749917-79-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (process for stereoselective synthesis of pentostatin aglycon and pentostatin via cyclization of dinitrile derivs. with amines)

RN 749917-70-2 CAPLUS

CN Carbamic acid, [(1S,2S)-1,2-dicyano-2-[[(1,1-dimethylethyl)diphenylsilyl]oxy]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 749917-71-3 CAPLUS

CN Butanedinitrile, 2-amino-3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 749917-79-1 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine, 8-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-3,6,7,8-tetrahydro-6-(3-nitrobenzoyl)-3-(phenylmethyl)-, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 749917-72-4P 749917-81-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(process for stereoselective synthesis of pentostatin aglycon and pentostatin via cyclization of dinitrile derivs. with amines)

RN 749917-72-4 CAPLUS

Absolute stereochemistry. Double bond geometry as shown.

RN 749917-81-5 CAPLUS
CN Imidazo[4,5-d][1,3]diazepine, 8-[[(1,1-dimethylethyl)diphenylsilyl]oxy]3,4,7,8-tetrahydro-3-(phenylmethyl)-, (8R)- (9CI) (CA INDEX NAME)

INVENTOR (S):

L18 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:33978 CAPLUS

DOCUMENT NUMBER: 140:94236

TITLE: Preparation of ring-expanded nucleosides and

nucleotides as virucides and bactericides Hosmane, Ramachandra S.; Sood, Ramesh K.

PATENT ASSIGNEE(S): Nabi, USA; University of Maryland Baltimore County

SOURCE: U.S., 51 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
US 6677310	B1	20040113	US 1999-295303	19990421		
US 2004077564	A1	20040422	US 2003-679429	20031007		
PRIORITY APPLN. INFO.:			US 1994-268570 B2	19940706		
			US 1995-518278 A3	19950823		
			US 1998-96614 B1	19980612		
			US 1999-290615 B2	19990413		
			US 1999-295303 A3	19990421		
OMITTED GOILD OF (O)	143 0 0 3 0	1 1 4 0 0 4 0 0 6				

OTHER SOURCE(S): MARPAT 140:94236

GI

AB The present invention relates to compns. comprising analogs of purine nucleosides containing a ring-expanded ("fat") heterocyclic ring, in place of purine, and an unmodified or modified sugar residue, pharmaceutically acceptable derivs. of such compns., as well as methods of use thereof. particular, these compns. may be utilized in the treatment of certain cancers, bacterial, fungal, parasitic, and viral infections, including, but not limited to, Acquired Immunodeficiency Syndrome (AIDS), hepatitis, Epstein-Barr and cytomegalovirus. The present invention relates to compns. comprising analogs of purine nucleosides containing a ring-expanded ("fat") heterocyclic ring, I (R1, R3, R5 = independently NH, NH2, O, OH, S, SH. NH-alkyl, N-alkyl, O-alkyl, S-alkyl, NH-aryl, O-aryl, S-aryl; R2, R4, R7, R8 = independently , H, alkyl, substituted Ph, heterocycle, aralkyl; R6 = H, alkyl, Ph, substituted Ph, heterocycle, aralkyl, glycosyl; U, X, Y, Z, W, J, K, L = C, N) in place of purine, and an unmodified or modified sugar residue, pharmaceutically acceptable derivs. of such compns., as well as methods of use thereof. In particular, these compns. may be utilized in the treatment of certain cancers, bacterial, fungal, parasitic, and viral infections, including, but not limited to, Acquired Immunodeficiency Syndrome (AIDS) and hepatitis.

6-Amino-6-methoxycarbonyl-4,5,7,8-tetrahydro-6H-imidazo[4,5,e]-[1,4]diazepine-5,8-dione was prepared as adenosine deaminase and guanase inhibitor and tested for its anti-retroviral and antibacterial activities. IT 155568-35-7P 155568-37-9P 155568-38-0P 159530-81-1P 159530-82-2P 162009-82-7P 169317-86-6P 169317-87-7P 216988-27-1P 224789-90-6P 244195-63-9P 398127-00-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of ring-expanded nucleosides and as virucides and bactericides) RN 155568-35-7 CAPLUS Imidazo[4,5-e][1,4]diazepine-5,8-dione, 3,4,6,7-tetrahydro-3,4,7-CN tris(phenylmethyl) - (9CI) (CA INDEX NAME)

$$Ph-CH_2$$
 $N$ 
 $CH_2-Ph$ 
 $CH_2-Ph$ 

RN 155568-37-9 CAPLUS
CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 2-bromo-3,4,6,7-tetrahydro-3,4-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 155568-38-0 CAPLUS
CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 2-bromo-3,4,6,7-tetrahydro-3,4,7-tris(phenylmethyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2$$
 $N$ 
 $N$ 
 $CH_2-Ph$ 
 $CH_2-Ph$ 

RN 159530-81-1 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-6-carboxylic acid, 6-amino-1,4,5,6,7,8-hexahydro-5,8-dioxo-, methyl ester (9CI) (CA INDEX NAME)

RN 159530-82-2 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-6-carboxylic acid, 1,4,5,6,7,8-hexahydro-6-methoxy-5,8-dioxo-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & H \\ & & & H \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 162009-82-7 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino-1- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 169317-86-6 CAPLUS

CN Imidazo[4,5-d][1,3]diazepin-5(1H)-one, 4,6,7,8-tetrahydro-8-hydroxy-1- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

RN 169317-87-7 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 1,4,6,7-tetrahydro-6-hydroxy-(9CI) (CA INDEX NAME)

RN 216988-27-1 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino-1- $\beta$ -D-ribofuranosyl-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$NH_2$$
 $NH_2$ 
 $NH_2$ 

# ●2 HCl

RN 224789-90-6 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8(1H,5H)-dione, 6-amino-1- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

RN 244195-63-9 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,6-diamine, 1,8-dihydro-1-[5-0[hydroxy[[hydroxy(phosphonooxy)phosphinyl]]-β-Dribofuranosyl]-8-imino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 398127-00-9 CAPLUS

CN Ethanol, 2-[(6,8-diamino-4-iminoimidazo[4,5-e][1,3]diazepin-1(4H)-yl)methoxy]- (9CI) (CA INDEX NAME)

$$NH_2$$
 $NH_2$ 
 $NH_2$ 
 $CH_2-O-CH_2-CH_2-OH$ 

IT 1122-28-7, 4,5-Dicyanoimidazole

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of ring-expanded nucleosides and as virucides and bactericides)

RN 1122-28-7 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 123124-90-3 CAPLUS CN 1H-Imidazole-4,5-dicarbonitrile, 1-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 139173-33-4 CAPLUS
CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 3,4,6,7-tetrahydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 139173-34-5 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 1,4,6,7-tetrahydro- (9CI) (CA INDEX NAME)

RN 139173-35-6 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 3,4,6,7-tetrahydro-3-(2,3,5-tri-0-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 139173-36-7 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 1,4,6,7-tetrahydro-1-(2,3,5-tri-0-benzoyl-β-D-ribofuranosyl) - (9CI) (CA INDEX NAME)

RN 139173-38-9 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 1,4,6,7-tetrahydro-1-β-Dribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 162009-80-5 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,6-diamine, 1,8-dihydro-8-imino-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 162009-81-6 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino-1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

RN 169317-84-4 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino- (9CI) (CA INDEX NAME)

RN 169317-88-8 CAPLUS

CN Methanesulfonic acid, trifluoro-, compd. with 1,6-dihydro-6-imino-1-(2,3,5tri-O-benzoyl-β-D-ribofuranosyl)imidazo[4,5-e][1,3]diazepine-4,8diamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 162009-81-6 CMF C32 H27 N7 O7

Absolute stereochemistry.

CM 2

CRN 1493-13-6 CMF C H F3 O3 S

RN 169317-91-3 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 3,4,6,7-tetrahydro-6-methoxy-3,4-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Ph-CH2} & \text{CH2-Ph} \\ \text{O} & & \\ \hline \\ \text{MeO} & & \\ \\ N & \\ N & \\ \\ N & \\ \end{array}$$

RN 169317-92-4 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 3,4,6,7-tetrahydro-6-hydroxy-3,4-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 216988-26-0 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8(1H,5H)-dione, 6-amino-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 216988-28-2 CAPLUS
CN 1H-Imidazole-4,5-dicarbonitrile, 1-β-D-ribofuranosyl- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ACCESSION NUMBER:
                         2000:741924 CAPLUS
                         133:305586
DOCUMENT NUMBER:
TITLE:
                         Methods of inducing cancer cell death and tumor
                         regression
INVENTOR (S):
                         Bishop, Walter R.; Brassard, Diana L.; Nagabhushan,
                         Tattanahalli L.
PATENT ASSIGNEE(S):
                         Schering Corporation, USA
                         PCT Int. Appl., 84 pp.
SOURCE:
                         CODEN: PIXXD2
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                        KIND
                               DATE
                                          APPLICATION NO.
                                                                 DATE
                                -----
                                           -----
                         ____
     WO 2000061145
                         A1
                               20001019 WO 2000-US9124
                                                                  20000406
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
             CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN,
             IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN,
             MX, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
             TZ, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                         US 1999-289255
     US 6316462
                               20011113
                         В1
                                                                   19990409
     CA 2364675
                                20001019
                                           CA 2000-2364675
                         AA
                                                                   20000406
     EP 1165078
                                          EP 2000-921765
                               20020102
                         A1
                                                                   20000406
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     BR 2000009670
                               20020115
                                           BR 2000-9670
                         Α
                                                                   20000406
     JP 2003529540
                         T2
                               20031007
                                            JP 2000-610478
                                                                   20000406
     NZ 514628
                                           NZ 2000-514628
                                                                   20000406
                         Α
                               20040130
     AU 783177
                                           AU 2000-42041
                         B2
                               20050929
                                                                   20000406
     ZA 2001008258
                                            ZA 2001-8258
                         Α
                               20030108
                                                                   20011008
PRIORITY APPLN. INFO.:
                                            US 1999-289255
                                                               A 19990409
                                                               W 20000406
                                            WO 2000-US9124
AB
     Methods are provided for treating cancer, comprising administering (1) a
     farnesyl protein transferase inhibitor in conjunction with (2) an addnl.
     Ras signaling pathway inhibitor to induce cancer cell death and tumor
     regression.
     53910-25-1, Pentostatin 109511-58-2, U0126
IT
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (methods of inducing cancer cell death and tumor regression with
        farnesyl protein transferase inhibitors in conjunction with Ras
        signaling pathway inhibitors and use of other antitumor agents)
RN
     53910-25-1 CAPLUS
CN
     Imidazo [4,5-d] [1,3] diazepin-8-ol, 3-(2-deoxy-\beta-D-erythro-
     pentofuranosyl)-3,4,7,8-tetrahydro-, (8R)- (9CI) (CA INDEX NAME)
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L18 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

RN109511-58-2 CAPLUS Butanedinitrile, bis[amino[(2-aminophenyl)thio]methylene]- (9CI) (CA CNINDEX NAME)

REFERENCE COUNT: 12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:785657 CAPLUS

DOCUMENT NUMBER: 130:38644

TITLE: Preparation of ring-expanded nucleosides and nucleotides as virucides and bactericides

INVENTOR(S): Hosmane, Ramachandra; Burns, Barry PATENT ASSIGNEE(S): University of Maryland, USA; Nabi

SOURCE: U.S., 24 pp., Cont.-in-part of U.S. Ser. No. 268,570,

abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5843912	A	19981201	US 1995-518278	19950823
US 2004077564	A1	20040422	US 2003-679429	20031007
PRIORITY APPLN. INFO.:			US 1994-268570 E	2 19940706
			US 1995-518278 A	3 19950823
			US 1998-96614 E	1 19980612
			US 1999-290615 E	2 19990413
			US 1999-295303 A	3 19990421

OTHER SOURCE(S): MARPAT 130:38644

GI

AB The present invention relates to compns. comprising analogs of purine nucleosides containing a ring-expanded ("fat") heterocyclic ring, I (R1, R3, R5 = independently NH, NH2, O, OH, S, SH. NH-alkyl, N-alkyl, O-alkyl, S-alkyl, NH-aryl, O-aryl, S-aryl; R2, R4, R7, R8 = independently , H, alkyl, substituted Ph, heterocycle, aralkyl; R6 = H, alkyl, Ph, substituted Ph, heterocycle, aralkyl, glycosyl, ; U, X, Y, Z, W, J, K, L =C, N) in place of purine, and an unmodified or modified sugar residue, pharmaceutically acceptable derivs. of such compns., as well as methods of use thereof. In particular, these compns. may be utilized in the treatment of certain cancers, bacterial, fungal, parasitic, and viral infections, including, but not limited to, Acquired Immunodeficiency Syndrome (AIDS) and hepatitis. 6-Amino-6-methoxycarbonyl-4,5,7,8tetrahydro-6H-imidazo[4,5,e]-[1,4]-diazepine-5,8-dione was prepared as adenosine deaminase and guanase inhibitor and tested for its anti-retroviral and antibacterial activities.

IT 159530-81-1P 159530-82-2P 162009-82-7P 169317-86-6P 169317-87-7P 216988-27-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

RN 159530-82-2 CAPLUS
CN Imidazo[4,5-e][1,4]diazepine-6-carboxylic acid, 1,4,5,6,7,8-hexahydro-6-methoxy-5,8-dioxo-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{MeO} - C & & \\ & & \\ & & \\ \end{array}$$

RN 162009-82-7 CAPLUS
CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino-1-β-Dribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 169317-86-6 CAPLUS
CN Imidazo[4,5-d][1,3]diazepin-5(1H)-one, 4,6,7,8-tetrahydro-8-hydroxy-1β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

RN 169317-87-7 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 1,4,6,7-tetrahydro-6-hydroxy-(9CI) (CA INDEX NAME)

RN 216988-27-1 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino-1- $\beta$ -D-ribofuranosyl-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# •2 HCl

IT 1122-28-7, 4,5-Dicyanoimidazole

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of ring-expanded nucleosides and as virucides and bactericides)

RN 1122-28-7 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 123124-90-3 CAPLUS CN 1H-Imidazole-4,5-dicarbonitrile, 1-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 139173-33-4 CAPLUS CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 3,4,6,7-tetrahydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 139173-34-5 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 1,4,6,7-tetrahydro- (9CI) (CA INDEX NAME)

RN 139173-35-6 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 3,4,6,7-tetrahydro-3-(2,3,5-tri-0-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 139173-36-7 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 1,4,6,7-tetrahydro-1-(2,3,5-tri-0-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

RN 139173-38-9 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 1,4,6,7-tetrahydro-1- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 162009-80-5 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,6-diamine, 1,8-dihydro-8-imino-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 162009-81-6 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino-1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

RN 169317-84-4 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino- (9CI) (CA INDEX NAME)

RN 169317-88-8 CAPLUS

CN Methanesulfonic acid, trifluoro-, compd. with 1,6-dihydro-6-imino-1-(2,3,5tri-O-benzoyl-β-D-ribofuranosyl)imidazo[4,5-e][1,3]diazepine-4,8diamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 162009-81-6 CMF C32 H27 N7 O7

Absolute stereochemistry.

CM 2

CRN 1493-13-6 CMF C H F3 O3 S

RN 169317-91-3 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 3,4,6,7-tetrahydro-6-methoxy-3,4-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Ph-CH_2 & CH_2-Ph \\ O & N \\ MeO & N \\ N \\ N \\ O \end{array}$$

RN 169317-92-4 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 3,4,6,7-tetrahydro-6-hydroxy-3,4-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

HO N 
$$CH_2-Ph$$

RN 216988-26-0 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8(1H,5H)-dione, 6-amino-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

Absolute stereochemistry.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

m 10/734,545

L18 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:878823 CAPLUS

DOCUMENT NUMBER: 123:286534

TITLE: Preparation of ring-expanded bases, nucleosides and

nucleotides as virucides, bactericides, fungicides,

and parasiticides.

INVENTOR(S):
Burns, Barry; Hosmane, Ramachandra

PATENT ASSIGNEE(S): USA

SOURCE: PCT Int. Appl., 84 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND DATE			APPLICATION NO.					DATE					
WO 9509175			A1 19950406		1	WO 1994-US10905				19940929							
	W: 1	AM, A'	r, AU,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	ES,	FI,	GB,	
	(	GE, H	U, JP,	ΚE,	KG,	KΡ,	KR,	ΚZ,	LK,	LT,	LU,	LV,	MD,	MG,	MN,	MW,	
	1	NL, N	o, NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SI,	SK,	ТJ,	TT,	UA,	UΖ,	VN	
	RW:	KE, M	W, SD,	SZ,	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,	LU,	
	I	MC, N	L, PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML,	MR,	NE,	SN,	
		TD, T	G														
CA	CA 2173116			AA 19950406 CA 1994-217			2173	116	19940929								
AU				A1 19950418 AU 1994-78445				5	19940929								
EP 724587			A1 19960807 EP 1994-929358					19940929									
EP	72458	7		B1		2002	0904										
	R: 2	AT, B	E, CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,	LI,	LU,	MC,	NL,	PT,	SE
EP	122710	03		A2		2002	0731	]	EP 2	002-3	1587			1:	9940	929	
EP	12271	03		<b>A</b> 3		2002	1016										
	R: 2																ΙE
AT	223428	8		E		2002	0915	7	AT 1:	994-9	9293	58		1	9940	929	
PT 724587			T 20030131				AT 1994-929358 PT 1994-929358				19940929						
ES	218284	47		Т3		2003	0316	1	ES 1:	994-9	9293	58		1:	9940	929	
PRIORIT	Y APPLI	N. IN	FO.:					1	US 1:	993-:	1282	12	7	A 1:	9930:	929	
								]	EP 1:	994-	9293	58	7	A3 1	9940	929	
								Ī	WO 1	994-T	JS10:	905	1	W 1	9940	929	
OTHER SOURCE(S):			MARI	PAT	123:	2865						,					

$$\begin{array}{c|c}
R^1 \\
\parallel & (R^8)_a \\
U & J \\
\downarrow & K(R^7)_a \\
R^3 = Y & \parallel \\
\downarrow & (R^4)_a & R^5
\end{array}$$

AB Title compds. [I; R1, R3, R5 = NH, NH2, O, OH, S, SH, alkoxy, alkylthio, alkylamino, alkylimino, (substituted) aryloxy, arylamino, arylthio,

Ι

GI

glycosylamino, glycosylimino, etc.; R2, R4, R6, R7, R8 = H, alkyl, (substituted) aryl, aralkyl, glycosyl, etc.; U, X, Y, Z, W, J, K, L = C, N, O, P, S; a = 0, 1] and related compds., were prepared Thus, 4,5-dicyanoimidazole, 1-O-acetyl-2,3,5-tri-O-benzoyl- $\beta$ -D-ribofuranose, hexamethyldisilazane, Me3SiCl, and F3CSO3H were stirred in MeCN in an ice water bath to give 94% 1-(2,3,5-tri-O-benzoyl- $\beta$ -D-ribofuranosyl)-4,5-dicyanoimidazole. The latter was refluxed overnight with guanidine hydrochloride and NaOMe in MeOH to give 40% 4,6,8-triimino-1- $\beta$ -D-ribofuranosylimidazo[4,5-e][1,3]diazepine. The latter inhibited adenosine deaminase with Ki = 3.85-4 + 10-4 M. 159530-81-1P 159530-82-2P 162009-80-5P

TT 159530-81-1P 159530-82-2P 162009-80-5P 162009-82-7P 169317-84-4P 169317-85-5P 169317-86-6P 169317-87-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of ring-expanded bases, nucleosides and nucleotides as virucides, bactericides, fungicides, and parasiticides)

RN 159530-81-1 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-6-carboxylic acid, 6-amino-1,4,5,6,7,8-hexahydro-5,8-dioxo-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & H \\ & & & & H \\ & & & & \\ H_2N & & & & \\ & & & & \\ MeO-C & & & M \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 159530-82-2 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-6-carboxylic acid, 1,4,5,6,7,8-hexahydro-6-methoxy-5,8-dioxo-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{MeO} - C & & \\ & & \\ & & \\ \end{array}$$

RN 162009-80-5 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,6-diamine, 1,8-dihydro-8-imino-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 162009-82-7 CAPLUS

CN Imidazo[4,5-e] [1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino-1- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 169317-84-4 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino- (9CI) (CA INDEX NAME)

RN 169317-85-5 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8(1H,5H)-dione, 6-amino- (9CI) (CA INDEX NAME)

RN 169317-86-6 CAPLUS

CN Imidazo[4,5-d][1,3]diazepin-5(1H)-one, 4,6,7,8-tetrahydro-8-hydroxy-1- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 169317-87-7 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 1,4,6,7-tetrahydro-6-hydroxy-(9CI) (CA INDEX NAME)

IT 139173-35-6P

RL: BYP (Byproduct); PREP (Preparation) (preparation of ring-expanded bases, nucleosides and nucleotides as virucides, bactericides, fungicides, and parasiticides)

RN 139173-35-6 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 3,4,6,7-tetrahydro-3-(2,3,5-tri-0-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 1122-28-7, 4,5-Dicyanoimidazole

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of ring-expanded bases, nucleosides and nucleotides as virucides, bactericides, fungicides, and parasiticides)

RN 1122-28-7 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile (9CI) (CA INDEX NAME)

IT 94619-73-5P 123124-90-3P 139173-33-4P 139173-34-5P 139173-36-7P 139173-38-9P

169317-88-8P 169317-91-3P 169317-92-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of ring-expanded bases, nucleosides and nucleotides as virucides, bactericides, fungicides, and parasiticides)

RN 94619-73-5 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile, 1-(2,3,5-tri-O-benzoyl-β-Dribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 123124-90-3 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile, 1-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 139173-33-4 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 3,4,6,7-tetrahydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 139173-34-5 CAPLUS
CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 1,4,6,7-tetrahydro- (9CI) (CA INDEX NAME)

RN 139173-36-7 CAPLUS
CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 1,4,6,7-tetrahydro-1-(2,3,5-tri-0-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 139173-38-9 CAPLUS

CN Imidazo[4,5-d][1,3]diazepine-5,8-dione, 1,4,6,7-tetrahydro-1-β-Dribofuranosyl- (9CI) (CA INDEX NAME)

RN 169317-88-8 CAPLUS

CN Methanesulfonic acid, trifluoro-, compd. with 1,6-dihydro-6-imino-1-(2,3,5tri-O-benzoyl-β-D-ribofuranosyl)imidazo[4,5-e][1,3]diazepine-4,8diamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 162009-81-6 CMF C32 H27 N7 O7

Absolute stereochemistry.

CM 2

CRN 1493-13-6 CMF C H F3 O3 S

RN 169317-91-3 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 3,4,6,7-tetrahydro-6-methoxy-3,4-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Ph-CH2} & \text{CH2-Ph} \\ \text{O} & & \\ \\ \text{MeO-N} & & \\ \\ \text{N} & & \\ \\ \text{O} & & \\ \end{array}$$

RN 169317-92-4 CAPLUS

CN Imidazo[4,5-e][1,4]diazepine-5,8-dione, 3,4,6,7-tetrahydro-6-hydroxy-3,4-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

HO N 
$$CH_2-Ph$$

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L18 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:273394 CAPLUS

DOCUMENT NUMBER: 122:214413

TITLE: A short synthesis of a novel ring-expanded purine and

its nucleoside analog containing the

imidazo[4,5-e][1,3]diazepine ring skeleton with

multiple amino substituents attached to the 7-membered

ring

AUTHOR(S): Wang, Lijuan; Bhan, Anila; Hosmane, Ramachandra S.;

Guiles, R. D.

CORPORATE SOURCE: Dep. of Chemistry and Biochemistry, Univ. of Maryland

Baltimore County, Baltimore, MD, 21228, USA

SOURCE: Nucleosides & Nucleotides (1994), 13(10), 2307-20

CODEN: NUNUD5; ISSN: 0732-8311

PUBLISHER: Dekker
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:214413

GΙ

$$NH_2$$
 $NH_2$ 
 $NH_2$ 

The synthesis of 4,6,8-triaminoimidazo[4,5-e][1,3]diazepine (I) and its nucleoside analog (II) are reported. The heterocycle was prepared in a single step by condensation of 4,5-dicyanoimidazole with guanidine. The 5,7-fused ring structure of I was distinguished from the other possible 5:5-fused isomer by preparing the 15N-labeled heterocycle (1\*) and exploring its 15N-lH coupling patterns in both 1H and 15N NMR spectra. These spectral patterns also enabled establishment of the triamino tautomeric form of I as assigned. Compound I, a novel ring-expanded ("fat") analog of purine, is anticipated to be planar and aromatic as predicted by mol. modeling. The 1-benzyl analog (III), a protocol for the ribosyl analog II, was similarly prepared from 1-benzyl-4,5-dicyanoimidazole. The nucleoside II was prepared by the modified Vorbrueggen ribosylation of I.

The position of ribosylation was unequivocally established by an unambiguous synthesis of II from condensation of 1-(2',3',5'-tri-O-benzoyl- $\beta$ -D-ribofuranosyl)-4,5-dicyanoimidazole (IV) with guanidine in a solution of sodium methoxide in methanol. The nucleoside IV was prepared by the Vorbrueggen ribosylation of 4,5-dicyanoimidazole.

IT 94619-73-5P 123124-90-3P 162009-79-2P

162009-80-5P 162009-81-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(a short synthesis of a novel ring-expanded aminopurine and nucleoside analog)

RN 94619-73-5 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile, 1-(2,3,5-tri-O-benzoyl-β-Dribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 123124-90-3 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile, 1-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 162009-79-2 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,6,8-triamine (9CI) (CA INDEX NAME)

RN 162009-80-5 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,6-diamine, 1,8-dihydro-8-imino-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$NH_2$$
 $NH_2$ 
 $NH_2$ 
 $CH_2-Ph$ 

RN 162009-81-6 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino-1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 162009-82-7P 162009-83-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(a short synthesis of a novel ring-expanded aminopurine and nucleoside analog)

RN 162009-82-7 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,8-diamine, 1,6-dihydro-6-imino-1-β-Dribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 162009-83-8 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,6,8-triamine-N6,5,7-15N3 (9CI) (CA INDEX NAME)

ΙT

1122-28-7, 4,5-Dicyanoimidazole
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with guanidine)

RN1122-28-7 CAPLUS

CN1H-Imidazole-4,5-dicarbonitrile (9CI) (CA INDEX NAME)

ANSWER 8 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:198331 CAPLUS

DOCUMENT NUMBER: 112:198331

TITLE: Imidazo[4,5-e][1,3]diazepine-4,6-dione. A novel

xanthine analog

AUTHOR(S): Bridson, Peter K.; Lambert, Steven J.

CORPORATE SOURCE: Dep. Chem., Memphis State Univ., Memphis, TN, 38152,

USĀ

SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999)

(1990), (1), 173-5

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:198331

GI

CONH<sub>2</sub>

CH<sub>2</sub>NHCON

N

R

NH

NH

NH

NH

II

AB Imidazolylcarbonylaminomethylimidazolecarboxamide I was treated with Ac20 in anhydrous dioxan to give 40% benzyldihydroimidazodiazepinedione II (R = PhCH), which on hydrogenolysis gave II (R = H).

IT 126921-91-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and debenzylation of)

RN 126921-91-3 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,6(1H,5H)-dione, 7,8-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

HN N CH2-Ph

IT 126921-83-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 126921-83-3 CAPLUS

CN Imidazo[4,5-e][1,3]diazepine-4,6(1H,5H)-dione, 7,8-dihydro- (9CI) (CA

INDEX NAME)